Calculations to Refine Beryllium's Equation of State

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Our current equation of state (EOS) for beryllium is based on experimental data and empirical models. This construction does not fully constrain the resulting EOS, and recently uncovered experimental results in the literature show slight disagreement with the established EOS of Be. Is this due to the original construction of the EOS, or are the original and newer experiments incompatible with each other? To help resolve this question, we turn to the third underpinning of a successful EOS, density functional theory (DFT) (see Fig. 1).

Figure 2 shows the calculated average phonon frequency θ_0 for Be in the hexagonal close packed (hcp) structure as a function of volume. This average phonon frequency provides a measure for how much thermal energy Be can absorb. How this measure changes with volume determines the thermal EOS and is quantified in the Grüneisen parameter Γ. The Grüneisen parameter is given by the (logarithmic) derivative of θ_0 with respect to the volume, which we obtain by first fitting our calculated θ_0 as a function of V.

Figure 3 compares the calculated Grüneisen parameter with that of the original EOS model. While the differences are reasonably small, a slight change in the model improves the agreement without destroying the good agreement obtained for other variables such as the cold curve (see Fig. 4).

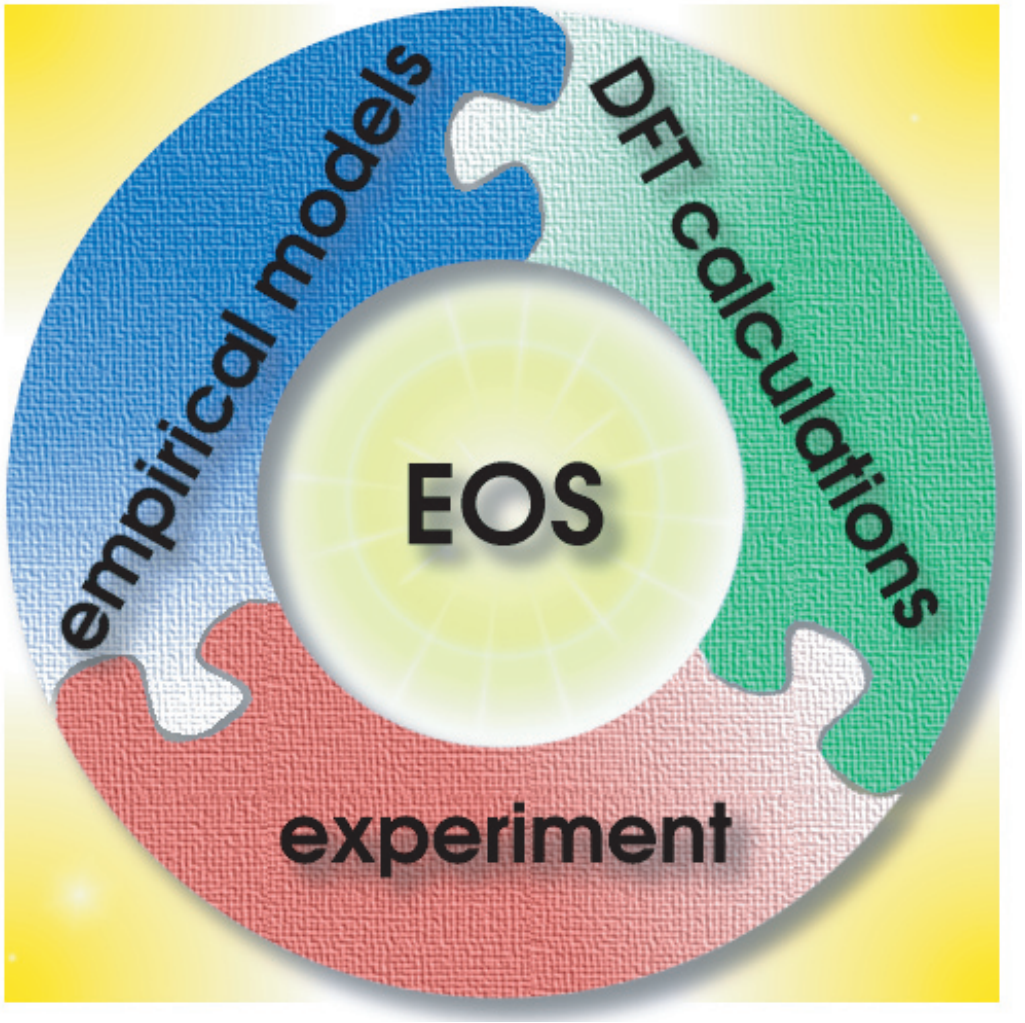

Figure 1—
The three components that contribute complementary data to an EOS—experiment, empirical models, and DFT calculations.

The average phonon frequencies shown here are from preliminary calculations using DFT. These calculations are now being systematically improved, the end goal being an EOS for Be that is consistent with all data available to us.

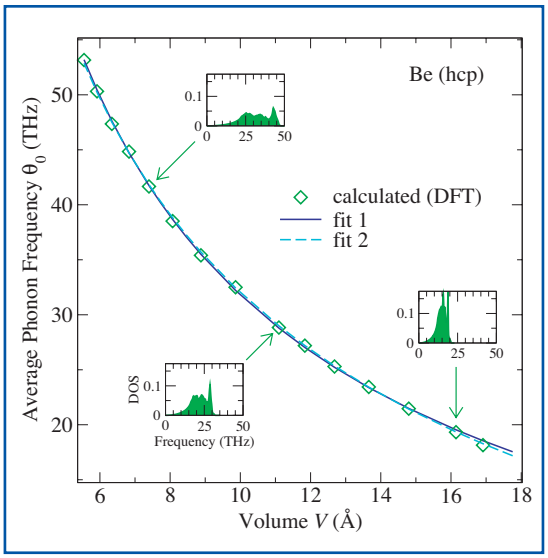

Figure 2—
Calculated average phonon frequency Θ_0 for Be in the hcp crystal structure as a function of volume. The functional form of the two fits give either a linear (fit 1) or a quadratic (fit 2) relation between the Grüneisen parameter Γ and the volume V.

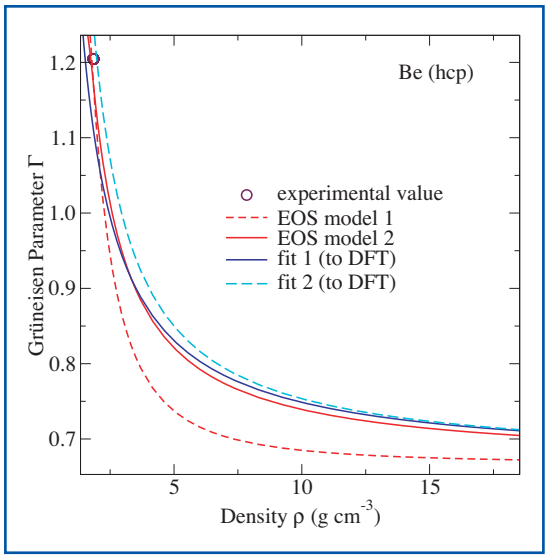

Figure 3—
Grüneisen parameter Γ for Be. The two fits to the DFT calculations lie very close to each other but differ somewhat from the old EOS model (model 1). A slight change in the model (now model 2) gives better agreement. All curves are forced to tend towards 2/3 with increasing density ρ.

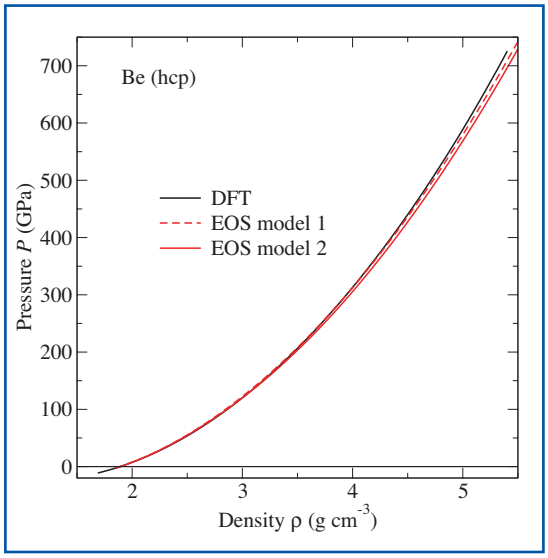

Figure 4—
Cold curves for Be. The curve calculated with DFT is in good agreement with both the original EOS model (model 1) as well as the model that was refit (model 2) to agree better with the calculated Grüneisen parameter.